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User's Manual for the FEHM Application— A Finite-element Heat- and Mass-transfer Code

by

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ABSTRACT

This document is a manual for the use of the FEHM application, a finite-element heat- and mass-transfer computer code that can simulate nonisothermal multiphase multicomponent flow in porous media. The use of this code is applicable to natural-state studies of geothermal systems and groundwater flow. The primary use of the FEHM application will be to assist in the understanding of flow fields and mass transport in the saturated and unsaturated zones below the proposed Yucca Mountain nuclear waste repository in Nevada. The equations of heat and mass transfer for multiphase flow in porous and permeable media are solved in the FEHM application by using the finite-element method. The permeabililty and porosity of the medium are allowed to depend on pressure and temperature. The code also has provisions for movable air and water phases and noncoupled tracers; that is, tracer solutions that do not affect the heat- and mass-transfer solutions. The tracers can be passive or reactive. The code can simulate two-dimensional, two-dimensional radial, or three-dimensional geometries. In fact, FEHM is capable of describing flow that is dominated in many areas by fracture and fault flow, including the inherently three-dimensional flow that results from permeation to and from faults and fractures. The code can handle coupled heat and mass-transfer effects, such as boiling, dryout, and condensation that can occur in the near-field region surrounding the potential repository and the natural convection that occurs through Yucca Mountain due to seasonal temperature changes. The code is also capable of incorporating the various adsorption mechanisms, ranging from simple linear relations to nonlinear isotherms, needed to describe the very complex transport processes at Yucca Mountain. This report outlines the uses and capabilities of the FEHM application, initialization of code variables, restart procedures, and error processing. The report describes all the data files, the input data, including individual input records or parameters, and the various output files. The system interface is described, including the software environment and installation instructions. Examples illustrating various aspects of the code are sprinkled throughout the report, and the final section demonstrates how to construct an input file, shows typical code execution, and gives three examples: heat conduction in a square, a reactive-transport problem, and Problem 5, Case A, of the DOE Code-comparison Project.

1.0 PURPOSE

This User's Manual documents the use of the finite-element heat- and mass-transfer (FEHM) application (Zyvoloski, et al. 1988).

2.0 DEFINITIONS AND ACRONYMS

2.1 Definitions

FEHM: finite-element heat- and mass-transfer code.

FEHMN: an earlier verion of FEHM designed specifically for the Yucca Mountain Site Characterization Project. Both versions are now equivalent, and the use of FEHMN has been dropped.

2.2 Acronyms

AVS: Advanced Visual Systems.

I/O: input/output.

LANL: Los Alamos National Laboratory.

UCD: unstructured cell data.

YMP: Yucca Mountain Site Characterization Project.

3.0 REFERENCES

Carslaw, H. S., and J. C. Jaeger. 1959. *Conduction of Heat in Solids*, 2nd edition. Clarendon Press.

Dash, Z. V., B. A. Robinson, and G. A. Zyvoloski. 1997. Software design, requirements, and validation for the FEHM application—a finite-element mass- and heat-transfer code. Los Alamos National Laboratory report LA-XXXX-MS.

Molloy, M. W. 1980. Geothermal reservoir engineering code comparison project. In *Proceedings of the Sixth Workshop on Geothermal Reservoir Engineering*. Stanford University.

Zyvoloski, G. A., Z. V. Dash, and S. Kelkar. 1988. FEHM: Finite element heat and mass transfer code. Los Alamos National Laboratory report LA-11224-MS.

Zyvoloski, G. A., Z. V. Dash, and S. Kelkar. 1991. FEHMN 1.0: Finite element heat and mass transfer code. Los Alamos National Laboratory report LA-12062-MS.

Zyvoloski, G. A., and Z. V. Dash. 1991. Software verification report FEHMN version 1.0. Los Alamos National Laboratory report LA-UR-91-609.

Zyvoloski, G. A., and B. A. Robinson. 1995. Models and methods summary for the GZSOLVE application. Los Alamos National Laboratory software document ECD-97.

Zyvoloski, G. A., B. A. Robinson, Z. V. Dash, and L. L. Trease. 1997. Summary of models and methods for the FEHM application—a finite-element mass- and heat-transfer code. Los Alamos National Laboratory report LA-XXXX-MS.

4.0 PROGRAM CONSIDERATIONS

4.1 Program Options

The uses and capabilities of FEHM are summarized in Table I with reference to the macro input structure discussed in Section 6.0.

Table I. Capabilities of FEHM with macro command references

I. Mass and energy balances in porous media
   - A. Variable rock properties (**rock**)
   - B. Variable permeability (**perm**)
   - C. Variable thermal conductivity (**cond**)
   - D. Variable fracture properties, dual porosity, and dual porosity/dual permeability (**dual, dpdp**)

II. Multiple components available
   - A. Air-water isothermal mixture available (**airwater**), fully coupled to heat and mass transfer (**ngas**)
   - B. Up to 10 solutes with chemical reactions between each (**trac, rxn)**
   - C. Several different capillary pressure models (**cap**)
   - D. Several different relative permeability models (**rlp**)

III. Equation of state flexibility inherent in code (**eos**)

IV. Psuedo-stress models available
   - A. Linear porosity deformation (**ppor**)
   - B. Gangi stress model (**ppor**)

V. Numerics
   - A. Finite element with multiple element capabilities (**elem**)
   - B. Short form input methods available (**coor, elem**)
   - C. Flexible properties assignment (**zone**)
   - D. Flexible solution methods
     1. Upwinding, implicit solution available (**ctrl**)
     2. Iteration control adaptive strategy (**iter**)
   - E. Finite volume geometry (**finv**)

VI. Flexible time step and stability control (**time**)

4.2 Initialization

The coefficient arrays for the polynomial representations of the density (crl, crv), enthalpy (cel, cev), and viscosity (cvl, cvv) functions are initialized to the values enumerated in the FEHM document "Models and Methods Summary" (Zyvoloski et al. 1997, Table III). Values for the saturation pressure and temperature function coefficients are also found in that document (Table IV). All other global array and scalar variables, with the exception of the variables listed below in Table II, whether integer or real, are initialized to zero.

Table II. Initial (default) values					
Variable	**Value**	**Variable**	**Value**	**Variable**	**Value**
aiaa	1.0	contim	1.0e+30	daymin	1.0e-05
daymax	30.0	g1	1.0e-06	g2	1.0e-06
g3	1.0e-03	iamx	500	ncntr	10000000
nicg	1	rnmax	1.0e+11	str	1.0
strd	1.0	tmch	1.0e-09	tmelt	-1.0e+12
upwgt	1.0	upwgta	1.0		

4.3 Restart Procedures

FEHM writes a restart file for each run. The name of the restart output file may be given in the input control file or as terminal input, or if unspecified, it will default to *fehmn.fin* (see Section 6.2.1). The file is used on a subsequent run by providing the name of the generated file (via control file or terminal) for the name of the restart input file. It is recommended that the name of the restart input file be modified to avoid confusion with the restart output file. For example, by changing the suffix to *.ini*, the default restart output file, *fehmn.fin*, would be renamed *fehmn.ini* and that file name placed in the control file or given as terminal input. Values from the restart file will overwrite any variable initialization prescribed in the input file. The initial time of simulation will also be taken from the restart file.

4.4 Error Processing

Due to the nonlinearity of the underlying partial differential equations, it is possible to produce an underflow or overflow condition through an unphysical choice of input parameters. More likely, the code will fail to converge or will produce results that are out of bounds for the thermodynamic functions. The code will attempt to decrease the time step until convergence occurs. If the time step drops below a prescribed minimum, the code will stop, writing a restart file. The user is encouraged to look at the input check file, which contains information regarding maximum and minimum values of key variables in the code. All error and warning messages will be sent to an output error file.

Table III provides additional information on errors that will cause FEHM to terminate.

Table III. Error conditions that result in program termination

Error condition	Error message
I/O file error	

Unable to open I/O file	`**** Error opening file fileid ****`
	.
	.
	.
	`****----------****`
	`****  JOB STOPPED  ****`
	`****----------****`

Coefficient storage file not found	`program terminated because coefficient storage file not found`
Optional rlp file not found	`relative perm file does not exist: stopping`
Optional input file not found	`ERROR nonexistant file filename` `STOPPED trying to use optional input file`
Unable to open optional input file	`ERROR opening filename` `STOPPED trying to use optional input file`
Unable to determine file prefix for AVS output files	`FILE ERROR: nmfil2 file: filename unable to determine contour file prefix`
Input deck errors	

Coordinate or element data not found	`****  COOR Required Input  ****`
	`-or-`
	`****  ELEM Required Input  ****`
	
	`****----------****`
	`****  JOB STOPPED  ****`
	`****----------****`

Invalid macro read	`**** error in input deck : char ****`

Invalid AVS keyword read for macro **cont**	`ERROR:READ_AVS_IO`
	`unexpected character string (terminate program execution)`
	`Valid options are shown:`
	.
	.
	.
	`The invalid string was:`
	`string`

Table III. Error conditions that result in program termination (continued)

Error condition	Error message
Invalid parameter values (macros using loop construct)	Fatal error - for array number *arraynum* macro - *macro* Group number - *groupnum* Something other than a real or integer has been specified -or- Line number - *line* Bad input, check this line
Invalid tracer input	** Using Old Input Enter Temperature Dependency Model Number: 1 - Van Hoff 2 - awwa model, see manual for details **
Invalid transport conditions	Fatal error. You specified a Henrys Law species with initial concentrations input for the vapor phase (icns = -2), yet the Henrys Constant is computed as 0 for species number *speciesnum* and node number *nodenum*. If you want to simulate a vapor-borne species with no interphase transport, then you must specify a gaseous species (icns = -1).
Invalid flag specified for diffusion coefficient calculation	ERROR -- Illegal Flag to concadiff Code Aborted in concadiff
Optional input file contains data for wrong macro	ERROR --> Macro name in file for macro *macroname* is *wrong_macroname* STOPPED trying to use optional input file
Invalid parameters set	
Dual porosity	**** check fracture volumes,stopping**** **** check equivalent continuum VGs ****
Noncondensible gas	cannot input ngas temp in single phase -or- ngas pressure lt 0 at temp and total press given max allowable temperature *temp* -or- ngas pressure gt total pressure i = *i* -or- ngas pressure lt 0.
Particle tracking	ERROR: Pcnsk in ptrk must be either always positive or always negative. Code aborted in set_ptrk.f

Table III. Error conditions that result in program termination (continued)

Error condition	Error message
Tracer	`ERROR: Can not have both particle tracking (ptrk) and tracer input (trac). Code Aborted in concen.f`
Insufficient storage	
Geometric coefficients	`program terminated because of insufficient storage`
Dual porosity	`***** n > n0, stopping **** `
Too many negative volumes or finite-element coefficients	`too many negative volumes: stopping` -or- `too many negative coefficients: stopping`
Unable to compute local coordinates	`iteration in zone did not converge, izone =` *zone* `please check icnl in macro CTRL`
Singular matrix in LU decomposition	`singular matrix in ludcmp`
Solution failed to converge	`timestep less than daymin` *timestep_number current_timestep_size current_simulation_time* -or- `Tracer Time Step Smaller Than Minimum Step Stop in resettrc`

5.0 DATA FILES

5.1 Control File (iocntl)

5.1.1 Content

The control file contains the names of the input and output files needed by the FEHM code. In addition to listing the I/O file names, the terminal (tty) output option and the user subroutine number are given. The control file provides the user an alternate means for inputting file names, terminal output option, and user subroutine number than through the terminal I/O. It is useful when long file names are used or when files are buried in several subdirectories, and it is also useful for automated program execution.

5.1.2 Use by program

The control file is an input file that provides the FEHM application with the names of the input and output files, the terminal output units, and the user subroutine number to be used for a particular run. The default control file name is *fehmn.files*. If the control file is found, it is read prior to problem initialization. If not present, terminal I/O is initiated, and the user is prompted for required information. A control file may use a name other than the default. This alternate control file name would be input during terminal I/O (see Section 6.1.1.1).

5.1.3 Auxiliary processing

N/A

5.2 Input File (inpt)

5.2.1 Content

The input file contains user-parameter initialization values and problem-control information. The form of the file name is *filen* or *filen*.*, where "*filen*" is a prefix used by the code to name auxiliary files and ".*" represents an arbitrary file extension. If a file name is not specified when requested during terminal I/O, the file *fehmn.dat* is the default. The organization of the file is described in detail in Section 6.2.

5.2.2 Use by program

The input file is an input file that provides the FEHM application with user-parameter initialization values and problem-control information. The input file is read during problem initialization.

5.2.3 Auxiliary processing

N/A

5.3 Geometry Data File (incoor)

5.3.1 Content

The geometry data file contains the mesh-element and coordinate data. This file can either be the same as the input file or a separate file.

5.3.2 Use by program

The geometry data file is an input file that provides the FEHM application with element and coordinate data. The geometry data file is read during problem initialization.

5.3.3 Auxiliary processing

N/A

5.4 Zone Data File (inzone)

5.4.1 Content

The zone data file contains the zone information (see macro **zone**). This file can either be the same as the input file or a separate file.

5.4.2 Use by program

The zone data file is an input file that provides the FEHM application with geometric-zone descriptions. The zone data file is read during problem initialization.

5.4.3 Auxiliary processing

N/A

5.5 Optional Input Files

5.5.1 Content

The optional input files contain user-parameter initialization values and problem-control information. The names of optional input files are provided in the main input file to direct the code to auxiliary files to be used for data input. Their use is described in detail in Section 6.2.

5.5.2 Use by program

The optional input file is an auxiliary input file that provides the FEHM application with user-parameter initialization values and problem-control information. The optional input files are read during problem initialization.

5.5.3 Auxiliary processing

N/A

5.6 Output File (iout)

5.6.1 Content

The output file contains the FEHM output. The file name is provided in the input control file or as terminal input, or it may be generated by the code from the name of the input file if terminal I/O is envoked. The generated name is of the form *filen.out*, where the "*filen*" prefix is common to the input file.

5.6.2 Use by program

The ouput file is an output file the FEHM application uses for general program time-step summary information. It is accessed throughout the program as the simulation steps through time.

5.6.3 Auxiliary processing

N/A

5.7 Read File (iread)

5.7.1 Content

The read file contains the initial values of pressure, temperature, saturation, and simulation time (the restart or initial state values). The naming convention is similar to that for the output file. The generated name is of the form *filen.ini*.

5.7.2 Use by program

The read file is an input file the FEHM application uses for program restarts. The read file is read during problem initialization.

5.7.3 Auxiliary processing

N/A

5.8 Write File (isave)

5.8.1 Content

The write file contains the final values of pressure, temperature, saturation, and simulation time for the run. This file can in turn be used as the read file in a restart run. The naming convention is similar to that for the output file. The generated name is of the form *filen.fin*.

5.8.2 Use by program

The write file is an output file the FEHM application uses for storing state data of the simulation. It is accessed at specified times throughout the program when state data should be stored.

5.8.3 Auxiliary processing

N/A

5.9 History Plot File (ishis)

5.9.1 Content

The history plot file contains data for time history plots of variables. The naming convention is similar to that for the output file. The generated name is of the form *filen.his*.

5.9.2 Use by program

The history plot file is an output file the FEHM application uses for storing time history data for pressure, temperature, flow, and energy output. It is accessed throughout the program as the simulation steps through time.

5.9.3 Auxiliary processing

This file is used to produce time history plots with the Browser (see Section 8.5).

5.10 Solute Plot File (istrc)

5.10.1 Content

The solute plot file contains time history data for solute concentrations at specified nodes. The naming convention is similar to that for the output file. The generated name is of the form *filen.trc*.

5.10.2 Use by program

The solute plot file is an output file the FEHM application uses for storing time history data for tracer output. It is accessed throughout the program as the simulation steps through time.

5.10.3 Auxiliary processing

This file is used to produce time history plots of tracers with the Browser (see Section 8.5).

5.11 Contour Plot File (iscon)

5.11.1 Content

The contour plot file contains the contour plot data. The naming convention is similar to that for the output file. The generated name is of the form *filen.con*.

5.11.2 Use by program

The contour plot file is an output file the FEHM application uses for storing contour data for pressure, temperature, flow, energy output, and tracer output. It is accessed at specified times throughout the program when contour data should be stored.

5.11.3 Auxiliary processing

N/A

5.12 Contour Plot File for dual or dpdp (iscon1)

5.12.1 Content

The dual or dpdp contour plot file contains the contour plot data for dual-porosity or dual-porosity/dual-permeability problems. The naming convention is similar to that for the output file. The generated name is of the form *filen.dp*.

5.12.2 Use by program

The dual or dpdp contour plot file is an output file the FEHM application uses for storing contour data for pressure, temperature, flow, energy output, and tracer output for dual-porosity or dual-porosity/dual-permeability problems. It is accessed at specified times throughout the program when contour data should be stored.

5.12.3 Auxiliary processing

N/A

5.13 Stiffness Matrix Data File (isstor)

5.13.1 Content

The stiffness matrix data file contains finite-element coefficients calculated by the code. It is useful for repeated calculations that use the same mesh, especially for large problems. The naming convention is similar to that for the output file. The generated name is of the form *filen.stor*.

5.13.2 Use by program

The stiffness matrix data file is both an input and an output file that the FEHM application uses for storing or reading finite-element coefficients calculated by the code. The stiffness matrix data file is read during problem initialization, if being used for input. It is accessed after finite-element coefficients are calculated, if being used for output.

5.13.3 Auxiliary processing

N/A

5.14 Input Check File (ischk)

5.14.1 Content

The input check file contains a summary of coordinate and variable information, suggestions for reducing storage, coordinates at which maximum and minimum values occur, and information about input for variables set at each node. The naming convention is similar to that for the output file. The generated name is of the form *filen.chk*.

5.14.2 Use by program

The input check file is an output file the FEHM application uses for writing a summary of the data initialization. The input check file is accessed after data initialization has been completed.

5.14.3 Auxiliary processing

N/A

5.15 Output Error File (ierr)

5.15.1 Content

The output error file contains any error or warning messages issued by the code during a run. The file is always named *fehmn.err* and will be found in the directory from which the problem was executed.

5.15.2 Use by program

The output error file is an output file the FEHM application uses for writing error or warning messages issued by the code during a run. It may be accessed at any time.

5.15.3 Auxiliary pProcessing

N/A

5.16 Advanced Visual Systems (AVS) Output Files

5.16.1 Content

The Advanced Visual Systems (AVS) output files contain geometry-based data that can be imported into AVS UCD (unstructured cell data) graphics routines. The AVS output files each have a unique file name indicating the section type, the data type, and the time step at which the files were created. These file names are automatically generated by the code and are of the form *fileprefix.NumberAVS_id*, where *fileprefix* is common to the contour-output-file prefix if defined, otherwise, it is the input-file prefix; *Number* is a value between 10001 and 99999; and *AVS_id* is a string denoting file content (see Table IV). In general, _head are header files, _geo is the geometry file, and _node with _mat, _sca, _vec, _con, _mat_dual, _sca_dual, _vec_dual, or _con_dual are the data selected for output. Currently all properties are node-based rather than cell-based.

Table IV. AVS file content tag

AVS_id	**File purpose**
_avs_log	Log file from AVS output routines
_geo	Geometry output file containing coordinates and cell information
_mat_head	AVS UCD header for material properties file
_mat_dual_head	AVS UCD header for material properties file for dual or dpdp
_sca_head	AVS UCD header for scalar-parameter values file
_sca_dual_head	AVS UCD header for scalar-parameter values file for dual or dpdp
_vec_head	AVS UCD header for vector-parameter values
_vec_dual_head	AVS UCD header for vector-parameter values for dual or dpdp
_con_head	AVS UCD header for solute concentration file
_con_dual_head	AVS UCD header for solute concentration file for dual or dpdp
_mat_node	Data output file with material properties
_mat_dual_node	Data output file with material properties for dual or dpdp
_sca_node	Data output file with scalar-parameter values (pressure, temperature, saturation)
_sca_dual_node	Data output file with scalar-parameter values (pressure, temperature, saturation) for dual or dpdp
_vec_node	Data output file with vector-parameter values (velocity)

Table IV. AVS file content tag (continued)	
AVS_id	**File purpose**
_vec_dual_node	Data output file with vector-parameter values (velocity) for dual or dpdp
_con_node	Data output file with solute concentration
_con_dual_node	Data output file with solute concentration for dual or dpdp

5.16.2 Use by program

The AVS output files are output files the FEHM application uses for storing geometry-based data for material properties, temperature, saturation, pressure, velocities, and solute concentrations in a format readable by AVS graphics. The log output file is created on the first call to the AVS write routines. It includes the code version number, date, and problem title. When output for a specified time step has been completed, a line containing the file-name prefix, time step, call number (this variable is 1 for the initial call and is incremented with each call to write AVS contour data) and time (days) is written. The header files, one for each type of data being stored, and the single geometry file are written during the first call to the AVS output routines. The node data files are written for each call to the AVS write routines at specified times throughout the program when contour data should be stored using AVS format.

5.16.3 Auxiliary processing

These files are used for visualization and analysis of data by AVS and to produce contour plots by the Browser (see Section 8.5).

To use these with AVS, the appropriate header file, geometry file, and data file for each node must be concatenated into one file of the form *filen.inp* (Fig. 1). This concatenation can be done with the script **fehm2avs** for a series of files with the same root *filen* or manually, for example:

```
cat filen.10001_head filen.10001_geo filen.10001_mat_node > filen.10001.inp
```

Once header and geometry have been merged with data files into a single AVS file, the data can be imported into AVS using the read_ucd module.

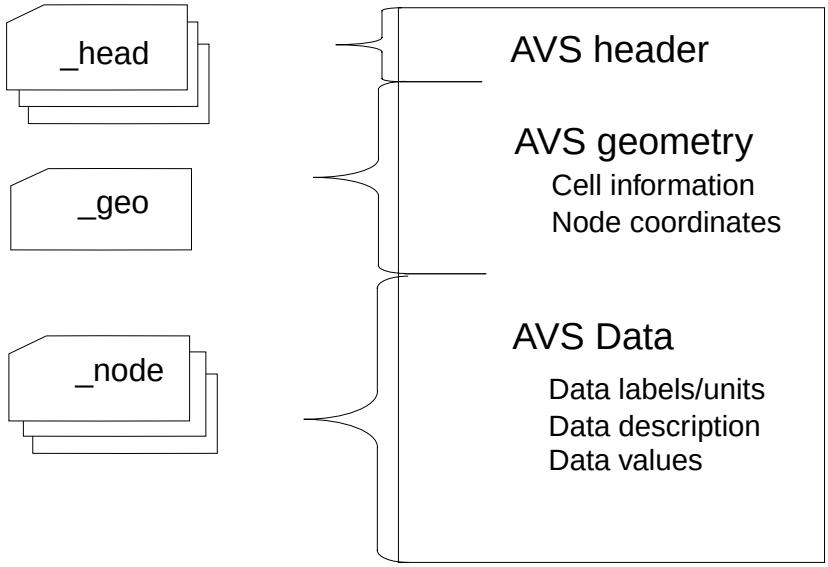

Figure 1. AVS UCD-formatted FEHM output files.